

ABSTRACT

A computer system comprising a first database containing records corresponding to a plurality of chemical compounds and records corresponding to biological information related to effects of the plurality of chemical compounds on biological systems and a second database containing records corresponding to a plurality of molecular targets. The computer system further comprises a third database containing records corresponding to tests of interaction between compounds in the first database and molecular targets in the second database, the tests including information on the effect that a compound from the plurality of compounds has on the interaction of a compound known to interact with a molecular target from the plurality of molecular targets and said molecular target. Means for setting an interaction test threshold corresponding to said effect and means for selecting the compound when its use results in a test meeting the interaction test threshold are also included in the computer system. A user interface is provided to allow a user to view the selected compound and to selectively view information from the first database, the second database, the third database as it relates to a compound record in the first database or as it relates to a molecular target in the second database.

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